



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:10 PM GMT

PDB ID : 1EF9  
Title : THE CRYSTAL STRUCTURE OF METHYLMALONYL COA DECARBOXYLASE COMPLEXED WITH 2S-CARBOXYPROPYL COA  
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Deposited on : 2000-02-07  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

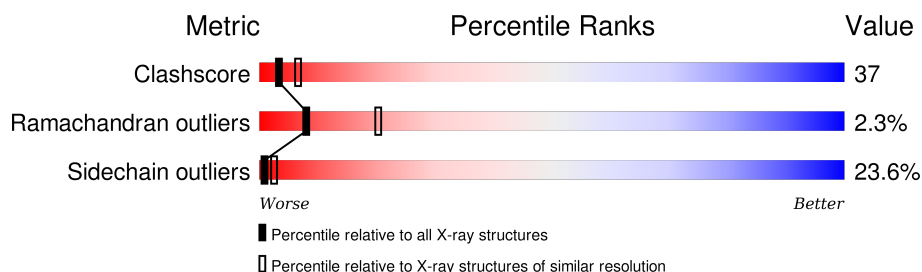
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2CP	A	270	X	-	-	-

## 2 Entry composition [i](#)

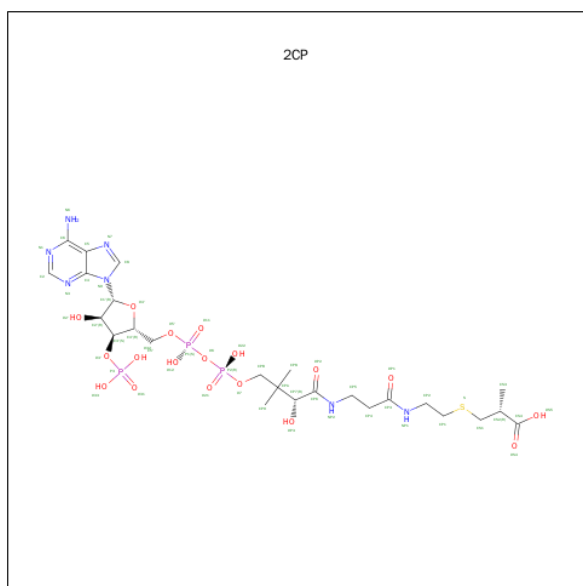
There are 2 unique types of molecules in this entry. The entry contains 2104 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHYLMALONYL COA DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	261	2050	1303	353	382	12	0	0	0

- Molecule 2 is 2-CARBOXYPROPYL-COENZYME A (three-letter code: 2CP) (formula:  $C_{25}H_{42}N_7O_{18}P_3S$ ).



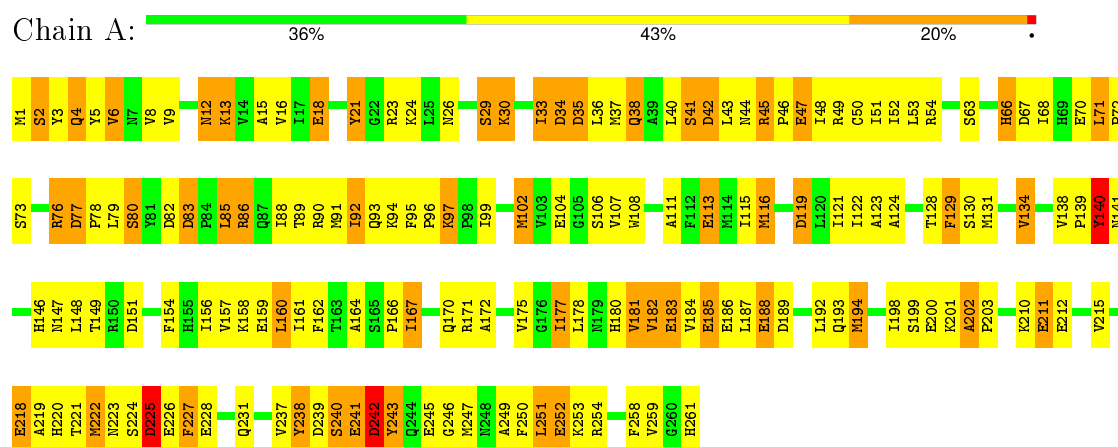
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	54	25	7	18	3	1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: METHYLMALONYL COA DECARBOXYLASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.70 Å   142.40 Å   89.70 Å 90.00°   109.20°   90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	87.0 (30.00-2.70)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2CP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.01	19/2091 (0.9%)	1.44	25/2828 (0.9%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	GLU	CD-OE2	5.87	1.32	1.25
1	A	226	GLU	CD-OE2	5.87	1.32	1.25
1	A	241	GLU	CD-OE2	5.74	1.31	1.25
1	A	186	GLU	CD-OE2	5.67	1.31	1.25
1	A	245	GLU	CD-OE2	5.60	1.31	1.25
1	A	70	GLU	CD-OE2	5.57	1.31	1.25
1	A	113	GLU	CD-OE2	5.54	1.31	1.25
1	A	200	GLU	CD-OE2	5.53	1.31	1.25
1	A	104	GLU	CD-OE2	5.48	1.31	1.25
1	A	252	GLU	CD-OE2	5.47	1.31	1.25
1	A	183	GLU	CD-OE2	5.40	1.31	1.25
1	A	212	GLU	CD-OE2	5.37	1.31	1.25
1	A	47	GLU	CD-OE2	5.30	1.31	1.25
1	A	211	GLU	CD-OE2	5.29	1.31	1.25
1	A	188	GLU	CD-OE2	5.25	1.31	1.25
1	A	185	GLU	CD-OE2	5.17	1.31	1.25
1	A	228	GLU	CD-OE2	5.12	1.31	1.25
1	A	218	GLU	CD-OE2	5.07	1.31	1.25
1	A	18	GLU	CD-OE2	5.06	1.31	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ASP	CB-CG-OD2	-8.63	110.53	118.30
1	A	227	PHE	CB-CG-CD2	8.04	126.43	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	A	189	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	A	77	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	A	83	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	119	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	151	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	42	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	225	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	67	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	119	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	97	LYS	C-N-CD	-6.44	106.42	120.60
1	A	242	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	238	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	A	34	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	227	PHE	N-CA-CB	5.89	121.21	110.60
1	A	67	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	90	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	239	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	242	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	238	TYR	CB-CG-CD1	5.31	124.18	121.00
1	A	77	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	227	PHE	CG-CD1-CE1	5.14	126.46	120.80
1	A	82	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2050	0	2058	155	0
2	A	54	0	38	7	0
All	All	2104	0	2096	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:HG2	1:A:238:TYR:CZ	2.00	0.95
1:A:116:MET:CE	1:A:177:ILE:HD13	2.05	0.85
1:A:78:PRO:HD2	1:A:238:TYR:CE1	2.12	0.84
1:A:1:MET:HG2	1:A:2:SER:H	1.42	0.82
1:A:116:MET:HE3	1:A:177:ILE:HD13	1.64	0.80
1:A:222:MET:HG2	1:A:227:PHE:CE2	2.18	0.79
1:A:76:ARG:HG3	1:A:77:ASP:N	1.96	0.79
1:A:72:PRO:HG2	1:A:78:PRO:HG3	1.64	0.79
1:A:50:CYS:C	1:A:51:ILE:HD13	2.02	0.79
2:A:270:2CP:H8	2:A:270:2CP:OP3	1.83	0.78
1:A:72:PRO:HG3	1:A:78:PRO:CB	2.18	0.73
1:A:68:ILE:HD12	2:A:270:2CP:N1	2.05	0.72
1:A:68:ILE:O	1:A:71:LEU:HB2	1.91	0.70
1:A:51:ILE:HG22	1:A:52:ILE:N	2.06	0.70
1:A:116:MET:CE	1:A:177:ILE:HG23	2.21	0.70
1:A:88:ILE:O	1:A:92:ILE:HG13	1.91	0.69
1:A:78:PRO:HG2	1:A:238:TYR:CE2	2.26	0.69
1:A:250:PHE:O	1:A:253:LYS:HG2	1.93	0.69
1:A:66:HIS:CE1	1:A:85:LEU:HD12	2.27	0.69
1:A:95:PHE:O	1:A:210:LYS:HE2	1.92	0.68
1:A:102:MET:HG2	1:A:187:LEU:HD21	1.75	0.68
1:A:72:PRO:HG3	1:A:78:PRO:CA	2.23	0.68
1:A:40:LEU:HD12	1:A:91:MET:HE2	1.76	0.67
1:A:157:VAL:O	1:A:161:ILE:HG13	1.95	0.67
1:A:1:MET:HG2	1:A:2:SER:N	2.10	0.67
1:A:51:ILE:HD13	1:A:51:ILE:N	2.08	0.66
1:A:40:LEU:HB2	1:A:91:MET:CE	2.25	0.66
1:A:68:ILE:HD13	1:A:250:PHE:CE1	2.31	0.66
1:A:259:VAL:HG11	1:A:261:HIS:CE1	2.32	0.65
1:A:76:ARG:HG3	1:A:77:ASP:H	1.60	0.64
1:A:116:MET:HE1	1:A:177:ILE:CG2	2.27	0.64
1:A:116:MET:HE1	1:A:177:ILE:HG23	1.78	0.64
1:A:13:LYS:HB3	1:A:47:GLU:O	1.98	0.64
1:A:253:LYS:HZ1	2:A:270:2CP:C2'	2.10	0.64
1:A:89:THR:O	1:A:93:GLN:HG3	1.97	0.64
1:A:223:ASN:ND2	1:A:225:ASP:HB2	2.13	0.63
1:A:72:PRO:CG	1:A:78:PRO:HG3	2.29	0.62
1:A:78:PRO:HG2	1:A:238:TYR:OH	2.01	0.61
1:A:38:GLN:HA	1:A:38:GLN:NE2	2.16	0.60
1:A:253:LYS:NZ	2:A:270:2CP:O2'	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:HA	1:A:183:GLU:OE1	2.00	0.60
1:A:1:MET:CG	1:A:2:SER:H	2.05	0.60
1:A:21:TYR:HB3	1:A:26:ASN:HA	1.84	0.60
1:A:250:PHE:O	1:A:253:LYS:N	2.33	0.59
1:A:40:LEU:HD12	1:A:91:MET:CE	2.32	0.59
1:A:21:TYR:HE2	1:A:29:SER:HG	1.51	0.58
1:A:94:LYS:O	1:A:96:PRO:HD3	2.03	0.58
1:A:237:VAL:O	1:A:240:SER:HB3	2.03	0.58
1:A:79:LEU:HD22	1:A:141:ASN:OD1	2.04	0.57
1:A:115:ILE:O	1:A:121:ILE:HD11	2.04	0.57
1:A:122:ILE:HD13	1:A:180:HIS:HB2	1.87	0.57
1:A:107:VAL:HG12	1:A:111:ALA:HB3	1.87	0.56
1:A:115:ILE:HD12	1:A:121:ILE:HD13	1.88	0.56
1:A:45:ARG:CB	1:A:46:PRO:HD2	2.37	0.55
1:A:16:VAL:HG22	1:A:52:ILE:HB	1.87	0.55
1:A:139:PRO:HG3	1:A:237:VAL:HB	1.88	0.55
1:A:72:PRO:HG3	1:A:78:PRO:HA	1.86	0.55
1:A:68:ILE:HD12	2:A:270:2CP:C6	2.37	0.55
1:A:78:PRO:CG	1:A:238:TYR:CZ	2.82	0.54
1:A:116:MET:HE1	1:A:177:ILE:HD13	1.84	0.54
1:A:146:HIS:O	1:A:149:THR:HG23	2.07	0.54
1:A:76:ARG:CG	1:A:77:ASP:H	2.19	0.53
1:A:68:ILE:HA	1:A:71:LEU:HD22	1.90	0.53
1:A:4:GLN:HG2	1:A:5:TYR:CG	2.43	0.53
1:A:129:PHE:CD1	1:A:129:PHE:N	2.75	0.53
1:A:201:LYS:O	1:A:203:PRO:HD3	2.08	0.53
1:A:130:SER:HB3	1:A:166:PRO:HA	1.90	0.53
1:A:242:ASP:OD1	1:A:258:PHE:HB3	2.09	0.53
1:A:21:TYR:HE2	1:A:29:SER:OG	1.91	0.53
1:A:139:PRO:O	1:A:140:TYR:O	2.27	0.53
1:A:175:VAL:HG23	1:A:177:ILE:HG13	1.90	0.52
1:A:51:ILE:CG2	1:A:52:ILE:N	2.72	0.52
1:A:72:PRO:CG	1:A:78:PRO:CG	2.88	0.52
1:A:30:LYS:HE3	1:A:34:ASP:OD1	2.10	0.52
1:A:51:ILE:HG22	1:A:52:ILE:H	1.73	0.52
1:A:66:HIS:HE1	1:A:85:LEU:HD12	1.72	0.52
1:A:222:MET:CG	1:A:227:PHE:CE2	2.91	0.51
1:A:3:TYR:OH	1:A:42:ASP:OD1	2.22	0.51
1:A:222:MET:SD	1:A:227:PHE:CD2	3.04	0.51
1:A:72:PRO:HG3	1:A:78:PRO:HB3	1.92	0.51
1:A:8:VAL:HG12	1:A:9:VAL:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HB2	1:A:91:MET:HE1	1.94	0.50
1:A:53:LEU:HD23	1:A:53:LEU:N	2.22	0.50
1:A:222:MET:SD	1:A:227:PHE:CE2	3.05	0.50
1:A:72:PRO:CG	1:A:78:PRO:CB	2.89	0.50
1:A:72:PRO:HG3	1:A:78:PRO:CG	2.41	0.50
1:A:115:ILE:HD12	1:A:121:ILE:CD1	2.41	0.49
1:A:113:GLU:HG2	1:A:113:GLU:O	2.11	0.49
1:A:86:ARG:NH1	1:A:113:GLU:OE1	2.28	0.49
1:A:259:VAL:HG11	1:A:261:HIS:NE2	2.27	0.49
1:A:21:TYR:CZ	1:A:24:LYS:HG3	2.48	0.49
1:A:72:PRO:CG	1:A:78:PRO:HB3	2.43	0.49
1:A:6:VAL:CG2	1:A:35:ASP:HB3	2.43	0.48
1:A:202:ALA:HA	1:A:203:PRO:HD2	1.66	0.48
1:A:68:ILE:CD1	1:A:250:PHE:CE1	2.97	0.47
1:A:243:TYR:O	1:A:246:GLY:N	2.42	0.47
1:A:88:ILE:O	1:A:88:ILE:HG13	2.13	0.47
1:A:95:PHE:CD2	1:A:99:ILE:HD11	2.50	0.47
1:A:68:ILE:HD13	1:A:250:PHE:CD1	2.50	0.47
1:A:15:ALA:CB	1:A:43:LEU:HD22	2.45	0.47
1:A:37:MET:HG3	1:A:88:ILE:HD12	1.96	0.46
1:A:181:VAL:O	1:A:181:VAL:HG12	2.14	0.46
1:A:38:GLN:NE2	1:A:38:GLN:CA	2.78	0.46
1:A:52:ILE:C	1:A:53:LEU:HD23	2.36	0.45
1:A:8:VAL:CG1	1:A:9:VAL:N	2.79	0.45
1:A:116:MET:HE1	1:A:177:ILE:HG21	1.98	0.45
1:A:21:TYR:HB3	1:A:26:ASN:HD22	1.81	0.45
1:A:18:GLU:HG3	1:A:54:ARG:HG3	1.97	0.45
1:A:253:LYS:NZ	2:A:270:2CP:C2'	2.79	0.45
1:A:68:ILE:HD13	1:A:250:PHE:HE1	1.79	0.45
1:A:160:LEU:HD11	1:A:167:ILE:HD13	1.98	0.45
1:A:77:ASP:HA	1:A:78:PRO:HD2	1.82	0.44
1:A:188:GLU:O	1:A:192:LEU:HG	2.17	0.44
1:A:242:ASP:OD2	1:A:258:PHE:HA	2.18	0.44
1:A:23:ARG:HH11	1:A:23:ARG:HD2	1.66	0.44
1:A:78:PRO:HD2	1:A:238:TYR:CZ	2.53	0.44
1:A:40:LEU:CB	1:A:91:MET:HE3	2.48	0.44
1:A:223:ASN:ND2	1:A:225:ASP:CB	2.80	0.44
1:A:138:VAL:HG13	1:A:139:PRO:HD2	1.99	0.44
1:A:139:PRO:HG3	1:A:237:VAL:CG1	2.48	0.44
1:A:240:SER:OG	1:A:241:GLU:N	2.51	0.43
1:A:223:ASN:HD21	1:A:225:ASP:CB	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:CG2	1:A:52:ILE:H	2.31	0.43
1:A:172:ALA:O	1:A:177:ILE:HB	2.18	0.43
1:A:211:GLU:O	1:A:215:VAL:HG23	2.19	0.43
1:A:250:PHE:C	1:A:253:LYS:H	2.18	0.43
1:A:71:LEU:HA	1:A:71:LEU:HD12	1.58	0.43
1:A:134:VAL:HG22	1:A:164:ALA:HB2	2.00	0.43
1:A:48:ILE:O	1:A:97:LYS:NZ	2.28	0.42
1:A:218:GLU:C	1:A:220:HIS:H	2.23	0.42
1:A:253:LYS:NZ	2:A:270:2CP:H2'	2.35	0.42
1:A:238:TYR:C	1:A:240:SER:H	2.22	0.42
1:A:251:LEU:HA	1:A:251:LEU:HD12	1.70	0.42
1:A:201:LYS:HG2	1:A:201:LYS:H	1.72	0.42
1:A:158:LYS:O	1:A:162:PHE:HB2	2.20	0.42
1:A:170:GLN:CD	1:A:170:GLN:H	2.23	0.42
1:A:33:ILE:HA	1:A:33:ILE:HD12	1.85	0.42
1:A:249:ALA:HA	1:A:254:ARG:HG2	2.01	0.42
1:A:15:ALA:HB3	1:A:51:ILE:HD12	2.02	0.42
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.93	0.41
1:A:49:ARG:CB	1:A:199:SER:HB2	2.50	0.41
1:A:146:HIS:O	1:A:148:LEU:N	2.53	0.41
1:A:63:SER:O	1:A:108:TRP:HD1	2.03	0.41
1:A:48:ILE:CG2	1:A:51:ILE:HD11	2.50	0.41
1:A:106:SER:OG	1:A:108:TRP:NE1	2.50	0.41
1:A:128:THR:C	1:A:129:PHE:CD1	2.93	0.41
1:A:79:LEU:HD13	1:A:140:TYR:HA	2.02	0.41
1:A:123:ALA:O	1:A:181:VAL:HA	2.20	0.41
1:A:40:LEU:CD1	1:A:91:MET:HE3	2.52	0.40
1:A:185:GLU:H	1:A:185:GLU:CD	2.24	0.40
1:A:194:MET:CG	1:A:198:ILE:HD11	2.51	0.40
1:A:37:MET:O	1:A:41:SER:HB2	2.21	0.40
1:A:12:ASN:HA	1:A:12:ASN:HD22	1.75	0.40
1:A:238:TYR:HA	1:A:238:TYR:HD2	1.79	0.40
1:A:249:ALA:O	1:A:253:LYS:N	2.54	0.40
1:A:124:ALA:HA	1:A:182:VAL:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/261 (99%)	212 (82%)	41 (16%)	6 (2%)	8	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	140	TYR
1	A	202	ALA
1	A	147	ASN
1	A	219	ALA
1	A	243	TYR

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/225 (100%)	172 (76%)	53 (24%)	1	2

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	4	GLN
1	A	6	VAL
1	A	12	ASN
1	A	13	LYS

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Mol	Chain	Res	Type
1	A	21	TYR
1	A	29	SER
1	A	30	LYS
1	A	33	ILE
1	A	35	ASP
1	A	36	LEU
1	A	38	GLN
1	A	41	SER
1	A	44	ASN
1	A	45	ARG
1	A	66	HIS
1	A	71	LEU
1	A	73	SER
1	A	76	ARG
1	A	80	SER
1	A	83	ASP
1	A	85	LEU
1	A	86	ARG
1	A	92	ILE
1	A	102	MET
1	A	116	MET
1	A	119	ASP
1	A	129	PHE
1	A	131	MET
1	A	134	VAL
1	A	140	TYR
1	A	154	PHE
1	A	156	ILE
1	A	160	LEU
1	A	167	ILE
1	A	171	ARG
1	A	177	ILE
1	A	178	LEU
1	A	181	VAL
1	A	182	VAL
1	A	184	VAL
1	A	193	GLN
1	A	194	MET
1	A	221	THR
1	A	222	MET
1	A	224	SER
1	A	225	ASP

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Mol	Chain	Res	Type
1	A	231	GLN
1	A	240	SER
1	A	242	ASP
1	A	247	MET
1	A	251	LEU
1	A	252	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	7	ASN
1	A	12	ASN
1	A	26	ASN
1	A	38	GLN
1	A	44	ASN
1	A	146	HIS
1	A	180	HIS
1	A	193	GLN
1	A	231	GLN
1	A	244	GLN
1	A	248	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	2CP	A	270	-	43,56,56	1.64	7 (16%)	53,83,83	1.87	13 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2CP	A	270	-	1/1/13/15	0/48/72/72	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	270	2CP	CP1-S	-4.49	1.64	1.81
2	A	270	2CP	CP2-NP1	-3.10	1.38	1.46
2	A	270	2CP	P3-O3'	-2.27	1.53	1.60
2	A	270	2CP	CP5-NP2	-2.05	1.41	1.46
2	A	270	2CP	O4'-C1'	2.26	1.44	1.41
2	A	270	2CP	CP3-NP1	2.38	1.39	1.33
2	A	270	2CP	CP6-NP2	4.85	1.43	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	270	2CP	CP5-NP2-CP6	-4.97	112.69	122.53
2	A	270	2CP	CP2-NP1-CP3	-3.84	115.24	122.79
2	A	270	2CP	CP4-CP3-NP1	-3.70	110.03	116.46
2	A	270	2CP	C2'-C3'-C4'	-3.11	97.45	103.29
2	A	270	2CP	N3-C2-N1	2.03	130.45	128.89
2	A	270	2CP	O6-P2-O7	2.58	109.77	102.94
2	A	270	2CP	O4'-C1'-N9	2.60	113.55	108.10
2	A	270	2CP	C2'-C1'-N9	2.77	118.52	114.29
2	A	270	2CP	O3'-C3'-C2'	2.79	122.37	111.51
2	A	270	2CP	O6-P1-O5'	3.03	110.97	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	270	2CP	O3'-C3'-C4'	3.31	122.97	109.99
2	A	270	2CP	CP8-CPA-CPB	3.44	112.96	108.50
2	A	270	2CP	CP2-CP1-S	4.46	130.78	114.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	270	2CP	CS2

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	270	2CP	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.